

Fate Report for Case # P-17-0023

Fate

Summary Statement

Fate P-17-0023

Summary

Statement: FATE:

Solid with MP = 95-97 °C (M)

log Kow = -0.90 (E)

S

> 10 g/L at 25 °C (E)

VP = 4.4E-2 torr at 25 °C (E)

BP = 209 °C

(E)

H = 1.15E-6 (E)

log Koc = 0.97 (E)

log Fish BCF = 0.50 (3)

(E)

log Fish BAF = -0.05 (1) (E)

POTW removal (%) = 0-25 via

possible biodeg

Time for complete ultimate aerobic biodeg = wk

Sorption to soils/sediments = low

Volatilization half-life from a

standard river = 570 hrs

Volatilization half-life from a standard lake

= 260 da

Atmospheric Oxidation Half-life = 120 hr via OH radical

PBT Potential: P3B1

*CEB FATE: Migration to ground water = rapid

Overall wastewater treatment removal is 0-25% based on analogous chemicals.

Sorption to sludge is low based on analogous chemicals.

Air Stripping (Volatilization to air) is low based on analogous chemicals and the estimated vapor pressure.

Removal by biodegradation

in wastewater treatment is negligible to moderate based on analogous chemicals and BIOWIN model estimates.

The aerobic aquatic

biodegradation half-life is weeks based on analogous chemicals.

The anaerobic aquatic biodegradation half-life is months to greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is low based on PCKOC model estimates and analogous chemicals.

Migration to groundwater is rapid based on the estimated water solubility and analogous chemicals.

PMN Material:

High Persistence

(P3) is based on the anaerobic biodegradation half-life.

Low

Bioaccumulation potential (B1) is based on analogous chemicals.

CBI: [REDACTED]

Fate Placeholder,

Assessor: Legacy

SMILES:

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	C2 H4 O4 S	C2 H4 O4 S1
Molecular Wt.:	124.12	124.11
%		
< 500:		
%		
< 1000:		

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:	95.00 - 97.00	Exp.			95.00
Boiling Point:			209	EPI	209.15
BP			@760		@760
Pressure:					
Vapor Pressure:			0.043	EPI	4.41e-002

Property	Measured Value	Method	Estimated Value	Method	EPI
Water Solubility:			407	EPI	
Log P:			-0.90		
Log Kow:					-0.90
Log Koc:					0.97
Log BCF:					3.1600
Henry's Law:					1.15e-006

pH:
pH
Comment:

Fate Analysis

Hydrolysis (t1/2, da):		Volatilization (t1/2) - River (hr):	568.3000	Volatilization (t1/2) - Lake (da):	262.2100
Atm Ox Potential (t1/2)OH (hr):	124.6900	Atm Ox Potential (t1/2)O3 (hr):		Atm Ox Potential (t1/2) Total (hr):	124.6900
MITI Linear:		MITI NonLinear:			
Biodeg Linear:	0.6900	Biodeg NonLinear:	0.7800		
Biodeg Survey ult:	WK	Biodeg Survey Prim:	DA-WK		
STP (% removal) Total:	1.9100	STP (% removal) Biodeg:	0.0900		
STP (% removal) Ads:	1.7500	STP (% removal) Air:	0.0700		

Rationales

Removal in Wastewater Treatment:
Atmospheric Oxidation:
Hydrolysis:
Photolysis:

Aerobic Biodegradation:
Anaerobic Biodegradation:
Sorption to Soil and Sediment:
Migration to Groundwater:
Persistence - Air:
Persistence - Water:
Volatilization from Water:
Soil:
Sediment:
Other:
Standard:
Bioaccumulation:

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
3	1	2	

Exposure-Based Testing

Exposure-Based Testing:

Fate Ratings

Removal in WWT/POTW

(Overall):

Removal in 0-25 WWT/POTW (Overall):
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Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	1	Low	Moderate	Strong	V. Strong	
	3	Extensive	Moderate	Low	Negligible	

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Stripping:						
Biodegradation Removal:	3-4	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	3-4	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	4	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio**Comments:**

Bio Fish log BAF = -0.05
Comments: (1).

Fate**Comments:**

Fate Overall wastewater

Comments: treatment removal is 0-25% based analogous chemicals.

Sorption to
sludge is low based on analogous chemicals.

Air Stripping

(Volatilization to air) is low based on analogous chemicals and the
estimated vapor pressure.

Removal by biodegradation in wastewater
treatment is negligible to moderate based on analogous chemicals and
BIOWIN model estimates.

The aerobic aquatic biodegradation half-life
is weeks based on analogous chemicals.

The anaerobic aquatic
biodegradation half-life is months to greater than months based on the
aerobic biodegradation half-life. The anaerobic biodegradation half-life
is projected to be greater or equal to the aerobic biodegradation
half-life.

Sorption to soil and sediment is low based on
PCKOC model estimates and analogous chemicals.

Migration to
groundwater is rapid based on the estimated water solubility and analogous
chemicals.

PMN Material:

High Persistence (P3) is based on the
anaerobic biodegradation half-life.

Low Bioaccumulation potential
(B1) is based on analogous chemicals.

Comments/Telephone Log

Artifact	Update/Upload Time
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